

IN THE CLAIMS:

1-10. (Canceled)

11. (Currently Amended) The method of claim ~~40~~ 21, wherein said physiological model is a mathematical model of said mammalian system comprising as operably linked components: ~~(i) differential~~ equations for calculating solubility and absorption of a test sample for one or more physiological segments of the mammal system of interest; and ~~(ii)~~ initial parameter values for the ~~differential~~ equations corresponding to physiological parameters and one or more selectively optimized adjustment parameters for one or more physiological segments of said mammal system of interest.

12. (Original) The method of claim 11, wherein said permeability data is derived from a cell-based assay.

13. (Original) The method of claim 12, wherein said solubility and said dissolution rate data is derived from a chemical-based assay.

14. (Original) The method of claim 11, wherein said mammalian system of interest is selected from the group consisting of the gastrointestinal tract, the eye, the nose, the lung, the skin, and the brain.

15. (Original) The method of claim 11, wherein said compound library is selected from the group consisting of a natural library, a synthetic library, and a combinatorial library.

16. (Original) The method of claim 11, wherein said physiological model is for a mammalian system selected from the group consisting of gastrointestinal tract, eye, nose, lung, skin, and blood brain barrier.

17. (Canceled)

18. (Currently Amended) The method of claim 11, which further comprises:

~~(iv) screening said secondary compound library by one or more~~ generating one or more predicted *in vivo* pharmacokinetic properties in addition to absorption; ~~(v) the absorption profile for the plurality of test samples;~~

selecting compounds by one or more of said ~~properties, and (vi) properties;~~ and
producing one or more compound libraries characterized by absorption, and one or more of said properties.

19. (Original) The method of claim 18, wherein said one or more properties in addition to absorption is selected from the group consisting of metabolism, toxicity and activity.

20. (Canceled)

21. (New) A method of screening a compound library or portion thereof by absorption, the method comprising:

providing a computer-implemented pharmacokinetic tool comprising an input/output system and a physiological model of a mammalian system of interest;

providing *in vitro* permeability and solubility data for a plurality of test samples from the compound library or portion thereof to the computer-implemented pharmacokinetic tool;

providing initial dose data to the computer-implemented pharmacokinetic tool;

generating a predicted *in vivo* absorption profile for each of the plurality of test samples with the computer-implemented pharmacokinetic tool; and

based on the generated absorption profiles, producing a secondary compound library comprising compounds having a desired absorption profile, whereby the compound library or portion thereof is screened by absorption.

22. (New) A method of screening a compound library or portion thereof by absorption, the method comprising:

providing a computer-implemented pharmacokinetic tool comprising an input/output system and a physiological model of a mammalian system of interest; the model comprises a selected adjustment parameter and the selected adjustment parameter comprises a value obtained by:

(i) assigning an initial value to the selected adjustment parameter;

(ii) inputting first data for a plurality of compounds into the model and running the model to generate output data;

(iii) comparing the output data with second data for the plurality of compounds;

(iv) selecting a new value for the selected adjustment parameter such that deviation of the comparison in step (iii) is reduced; and

(v) replacing the value of the selected adjustment parameter in the model with the new value selected in step (iv);

providing *in vitro* permeability and solubility data for a plurality of test samples from the compound library or portion thereof to the computer-implemented pharmacokinetic tool;

providing initial dose data to the computer-implemented pharmacokinetic tool;

generating a predicted *in vivo* absorption profile for each of the plurality of test samples with the computer-implemented pharmacokinetic tool; and

based on the generated absorption profiles, producing a secondary compound library comprising compounds having a desired absorption profile, whereby the compound library or portion thereof is screened by absorption.